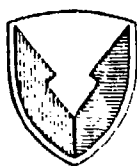US ARMY
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TECHNICAL REPORT BRL-TR-2729

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KINETIC MECHANISMS FOR PREMIXED, LAMINAR, STEADY STATE HYDROGEN/NITROUS OXIDE FLAMES

Terence P. Coffee

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20. ABSTRACT *(Continue on reverse side if necessary and identify by block number)*

A model has been developed for premixed, laminar, one-dimensional hydrogen/nitrous oxide flames. Results have been compared with a range of experimental data. The present model roughly reproduces the data, but inaccuracies still exist. Sensitivity and screening analyses have been used to indicate the additional experimental data needed to improve the model.

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I. INTRODUCTION

This report pertains to

~~We are interested here in the~~ detailed kinetics governing premixed, laminar, one-dimensional hydrogen, nitrous oxide flames. ~~Our~~ The long range goal is to understand the kinetics governing propellant decomposition, where nitrogen chemistry is important. Hydrogen/nitrous oxide flames are the simplest case of a flame controlled by nitrogen chemistry.

Controlled only by

This flame has previously been modeled by Cattolica et. al.[1] However, their model was compared only with one set of experimental profiles, a stoichiometric flame strongly stabilized on a porous plug flat flame burner. The model considered here is compared with a wider range of experimental data. We conclude that the basic mechanism is understood, but indicate where there are uncertainties in the model and the type of experimental data needed to resolve these uncertainties.

II. NUMERICAL PROCEDURE

The governing equations for the chemical species and the temperature are given in Ref. 2. These equations are integrated in time, using a finite element method, until the steady-state solution is obtained.[3-5]

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[1] R. Cattolica, M. Smooke, and A. Dean, "A Hydrogen-Nitrous Oxide Flame Study," Western States Section of the Combustion Institute, Paper WSS/CI 82-95, 1982.

[2] T.P. Coffee and J.M. Heimerl, "Transport Algorithms for Premixed, Laminar, Steady-State Flames," Combustion and Flame, Vol. 43 pp. 273-289, 1981.

[3] T.P. Coffee and J.M. Heimerl, "A Method for Computing the Flame Speed for a Laminar, Premixed, One Dimensional Flame," BRL Technical Report ARBRL-TR-02212, January 1980 (AD A082803).

[4] J.M. Heimerl and T.P. Coffee, "The Detailed Modeling of Premixed, Laminar, Steady-State Flames. I. Ozone," Combustion and Flame, Vol. 39, pp. 301-315, 1980.

[5] T.P. Coffee and J.M. Heimerl, "A Computer Code for the Solution of the Equations Governing a Laminar, Premixed, One-Dimensional Flame," BRL Memorandum Report ARBRL-MR-03165, April 1982 (AD A114041).

Besides the kinetics information, thermodynamic and transport data are required. The thermodynamic properties are obtained using the polynomial fits of Gordon and McBride.[6] The molecular parameters σ, ϵ/κ, and μ for the hydrogen/oxygen species are from Warnatz.[7] The parameters for the nitrogen species are from Svehla.[8] The polarizabilities are from Reid and Sherwood.[9] These are used to compute the individual species thermal conductivities and the binary diffusion coefficients. The multicomponent mass fluxes ($\rho\, Y_i\, V_i$) and heat flux (q) are computed using transport Method VI from Ref. 2.

III. KINETIC SCHEME

The forward reactions used in this paper are listed in Table 1. The rates of the back reactions are computed from the forward rate coefficients and the equilibrium constant for the reaction.

The hydrogen/oxygen scheme (the first 11 reactions) is taken from Warnatz.[7] Most of the nitrogen chemistry rate coefficients are from a recent review by Hanson and Salimian.[10] This review did not include reaction 20, which is taken from an earlier critical review by Baulch et. al.[11] The reverse rate coefficient for reaction 15 is discussed by Hanson and Salimian,

[6]S. Gordon and B.J. McBride, "Computer Program for Calculation of Complex Equilibrium Compositions, Rocket Performance, Incident and Reflected Shocks and Chapman-Jouguet Detonations," NASA-SP-273, 1971 (1981 program version).

[7]J. Warnatz, "The Structure of Laminar Alkane-, Alkene-, and Acetylene Flames," 18th International Combustion Symposium, The Combustion Institute, pp. 369-384, 1981.

[8]R.A. Svehla, "Estimated Viscosities and Thermal Conductivities of Gases at High Temperatures," NASA Technical Report R-132, Lewis Research Center, Cleveland, OH, 1962.

[9]R.C. Reed and J.K. Sherwood, The Properties of Gases and Liquids, 2nd edition, McGraw-Hill, NY, 1966.

[10]R.K. Hanson and S. Salimian, "Survey of Rate Constants in the N/H/O/ System," High Temperature Gasdynamics Laboratory, Stanford University, August 1983.

[11]D.L. Baulch, D.D. Drysdale, and D.G. Horne, Evaluated Kinetic Data for High Temperature Reactions, Vol. 2, London: Butterworths, 1973.

but the experiments to determine this show large differences, so no recommendation is made. Nip[12] is the only one to measure directly the forward rate coefficient for reaction 15, so we use this expression, but with the understanding that these values are not well determined.

The third body efficiencies for the hydrogen/oxygen system are from Warnatz. We treat NO like N_2 or O_2 and N_2O like CO_2. The efficiencies for reaction 20 are chosen to be the same as for reaction 4. The efficiencies for reaction 16 are estimated from data given by Baulch et. al.[11] This information is not accurately known, and the values used here are not much more than guesses.

TABLE 1. REACTIONS IN THE H_2/N_2O SYSTEM[a]

Reaction		A^b	B	C	Ref.
1. $OH + H_2$	$\rightarrow H_2O + H$	$1.00E+08^c$	1.60	1660	7
2. $H + O_2$	$\rightarrow OH + O$	$1.20E+17$	-.91	8340	7
3. $O + H_2$	$\rightarrow OH + H$	$1.50E+07$	2.00	3800	7
4. $H + O_2 + M'$	$\rightarrow HO_2 + M'$	$2.00E+18$	-.80	0	7
5. $H + HO_2$	$\rightarrow OH + OH$	$1.50E+14$	0.00	505	7
6. $H + HO_2$	$\rightarrow H_2 + O_2$	$2.50E+13$	0.00	349	7
7. $OH + HO_2$	$\rightarrow H_2O + O_2$	$2.00E+13$	0.00	0	7
8. $O + HO_2$	$\rightarrow OH + O_2$	$2.00E+13$	0.00	0	7
9. $H + H + M''$	$\rightarrow H_2 + M''$	$1.80E+18$	-1.00	0	7
10. $H + H + H_2$	$\rightarrow H_2 + H_2$	$9.70E+16$	-.60	0	7
11. $OH + OH$	$\rightarrow O + H_2O$	$1.50E+09$	1.14	0	7
12. $N_2O + O$	$\rightarrow NO + NO$	$6.92E+13$	0.00	13400	10
13. $N_2O + O$	$\rightarrow N_2 + O_2$	$1.00E+14$	0.00	14100	10
14. $N_2O + H$	$\rightarrow N_2 + OH$	$7.59E+13$	0.00	7600	10
15. $N_2O + H$	$\rightarrow NO + NH$	$1.90E+14$	0.00	17360	12

[12]W.S. Nip, Ph.D. thesis, University of Toronto, Toronto, Canada, 1974, as referenced by ref. 1 and ref. 10.

TABLE 1.   REACTIONS IN THE H_2/N_2O SYSTEM[a] (Con't)

		A	B	C	
16. $N_2O + M'''$	$\rightarrow N_2 + O + M'''$	6.92E+23	-2.50	32710	10
17. $NO + H$	$\rightarrow N + OH$	1.70E+14	0.00	24560	10
18. $NO + O$	$\rightarrow N + O_2$	3.80E+09	1.00	20620	10
19. $O + N_2$	$\rightarrow N + NO$	1.82E+14	0.00	38370	10
20. $NO + H + M'$	$\rightarrow HNO + M'$	5.40E+15	0.00	-300	11
21. $HNO + H$	$\rightarrow NO + H_2$	1.26E+13	0.00	2000	10
22. $HNO + OH$	$\rightarrow NO + H_2O$	1.26E+12	.50	1000	10
23. $HNO + O$	$\rightarrow NO + OH$	5.00E+11	.50	1000	10
24. $NH + H$	$\rightarrow N + H_2$	5.00E+13	0.00	1000	10
25. $NH + OH$	$\rightarrow N + H_2O$	5.00E+11	.50	1000	10
26. $NH + O$	$\rightarrow N + OH$	6.31E+11	.50	4000	10
27. $NH + O$	$\rightarrow NO + H$	6.31E+11	.50	0	10

[a] $[M]$ = total concentration; $[M'] = 0.4[NO] + 1.5[N_2O] + [H_2] + 0.4[O_2] + 6.5[H_2O] + 0.4[N_2] + 0.35[Ar]$; $[M''] = 0.4[NO] + 1.5[N_2O] + 0.4[O_2] + 6.5[H_2O] + 0.4[N_2] + 0.35[Ar]$; $[M'''] = [NO] + 5.0[N_2O] + [H_2] + [O_2] + 5.0[H_2O] + [N_2] + [Ar]$.

[b] A is in units of $cm^3\ mol^{-1}\ s^{-1}$ and $cm^6\ mol^{-2}\ s^{-1}$, $k=AT^B exp(-C/T)$.

[c] $1.00E+08 = 1.00 \times 10^8$.

IV.   COMPARISON WITH EXPERIMENTAL DATA

Relatively few measurements of burning velocity have been made for hydrogen/nitrous oxide flames. The most complete set is due to Duval and Van Tiggelen.[13] A selection of the flames measured is given in Table 2. One additional flame from Parker and Wolfhard[14] (50% H_2 and 50% N_2O) has been included. X represents the mole fraction of a species, and the stoichiometric coefficient $\phi = X_{H2}/X_{N20}$. These are atmospheric pressure flames with an

[13]A. Duval and P.J. Van Tiggelen, "Kinetical Study of Hydrogen-Nitrous Oxide Flames," Bull. Acad. Roy. Belges, Vol 53, pp. 366-402, 1967.

cold gas temperature of 290K. The burning velocities were measured using the schlieren cone method. The table includes the experimental burning velocity S_X, the model burning velocity S_M, and the percent difference $100(S_M - S_X)/S_X$. With one exception, the model burning velocities are uniformly lower than the experimental values.

The measurement of burning velocities has been critically reviewed by Andrews and Bradley.[15] In burner methods of measurement, the gas velocity normal to the flame is measured either directly or indirectly. The area of the flame must also be determined. Then the burning velocity can be derived.

Andrews and Bradley discuss a number of possible difficulties with this procedure. The main problem arises from the thickness of the flame. The position within the flame at which the flame area is measured affects the results. Andrews and Bradley recommend using correction factors to reference the flame back to the cold gas surface. They argue that burner methods normally underestimate the burning velocity.

More recently, Dixon-Lewis and Islam have studied burning velocity measurement using burner techniques.[16] They note that because of flow divergence, the derived burning velocity will be less for a plane near the hot side of the flame. They then show that to obtain accurate results the burning velocity must be referred to some position near the hot end of the flame. To obtain the gas velocity near the hot end of the flame, they recommend particle tracking.

Duval and Van Tiggelen did not use particle tracking, and it is difficult to determine an appropriate correction to their data. As a fairly simple check, we note that they used the same apparatus to measure the burning

[14]W.G. Parker and H.G. Wolfhard, "Some Characteristics of Flames Supported by NO and NO2," 4th International Combustion Symposium, The Combustion Institute, pp. 420-428, 1953.

[15]G.E. Andrews and D. Bradley, "Determination of Burning Velocities: A Critical Review," Combustion and Flame, Vol 18, pp. 133-153, 1973.

[16]G. Dixon-Lewis and S.M. Islam, "Flame Modelling and Burning Velocity Measurement," 19th International Combustion Symposium, The Combustion Institute, pp. 283-291, 1982.

velocities for methane/air flames.[17] The model for methane/air flames is better understood than for hydrogen/nitrous oxide flames, though it is not completely validated.[7,18,19] Table 3 compares the measurements of Burke and Van Tiggelen[17] with the model of Ref. 19. The model burning velocities seem too high for slower flames and slightly low for faster flames. Using this as an analogy, it seems likely that the hydrogen/nitrous oxide model does result in burning velocities that are somewhat too low.

Dixon-Lewis has measured burning velocities for very slow hydrogen/ nitrous oxide flames using an Egerton-Powling flat flame burner and particle tracking.[20] Some typical values are given in Table 4. The last flame in Table 4 is from another paper,[21] where species profiles were also measured. The burning velocities are referenced to the initial temperature of 400K. As before, the model burning velocites are slower except for the very rich case.

Dixon-Lewis and Islam measured the temperature profile and the N_2O, H_2, and N_2 profiles through a flame using thermocouples and quartz probes. The results for H_2 and temperature are given in figure 1. The model temperature profile is slightly steeper than the measured profile, reflecting the higher burning velocity. The H_2 profile shows similar differences. The other two species profiles are similar to H_2. In general, if the burning velocity is accurate, the temperature and major species profiles will also be accurate.[19]

[17]R. Burke and A. Van Tiggelen, "Kinetics of Laminar Premixed Methane-Oxygen-Nitrogen Flames," Bull. Soc. Chim. Belges, Vol 74, pp. 426-449, 1965.

[18]G. Dixon-Lewis, "Aspects of the Kinetic modeling of Methane Oxidation in Flames," 1st Specialists Meeting (International) of the Combustion Institute, France, pp. 284-289, 1981.

[19]T.P. Coffee, "Kinetic Mechanisms for Premixed, Laminar, Steady State Methane/Air Flames," Combustion and Flame Vol 55, pp. 161-170, 1984.

[20]G. Dixon-Lewis, "Stability of Hydrogen- Nitrous Oxide-Nitrogen Flames on a Flat Flame Burner," Combustion and Flame, Vol 8, pp. 85-87, 1964.

[21]G. Dixon-Lewis and S.M. Islam, "Some Reactions of Hydrogen Atoms and Simple Radicals at High Temperatures," 10th International Combustion Symposium, The Combustion Institute, pp. 495-502, 1965.

TABLE 2. BURNING VELOCITIES - DUVAL AND VAN TIGGELEN

ϕ	X_{H2}	X_{N2O}	X_{N2}	S_X	S_M	% Diff
.67	.2000	.3000	.5000	35	32.4	− 7
	.2300	.3450	.4250	65	48.1	−26
	.2800	.4200	.3000	113	80.7	−40
1.00	.2125	.2125	.5750	32	31.0	− 3
	.2500	.2500	.5000	65	51.1	−21
	.3500	.3500	.3000	156	121.6	−22
	.5000	.5000	.0000	390	255.5	−34
1.86	.3250	.1750	.5000	24	29.0	21
	.3900	.2100	.4000	69	58.1	−16
	.4550	.2450	.3000	129	96.3	−25

TABLE 3. BURNING VELOCITIES - METHANE FLAMES - BURKE AND VAN TIGGELEN

ϕ	X_{CH4}	X_{O2}	X_{N2}	S_X	S_M	% Diff
1.00	.1000	.2000	.7000	32	44.2	38
1.00	.1567	.3133	.5300	128	121.4	− 5
1.00	.1750	.3500	.4750	159	144.3	− 9

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TABLE 4. BURNING VELOCITIES – DIXON-LEWIS

ϕ	X_{H2}	X_{N2O}	X_{N2}	S_X	S_M	% Diff
.88	.1247	.1421	.7332	12.4	9.5	-23
.96	.1263	.1311	.7426	11.0	8.8	-20
1.00	.1269	.1269	.7462	9.9	8.5	-14
1.77	.2146	.1210	.6644	9.3	11.3	22

Recently, Cattolica et. al. have made profile measurements using laser techniques on a 50% H_2, 50% N_2O flame.[1] The flame is strongly stabilized on a flat flame burner. The temperature of the burner is approximately 1000K and the gas flow from the burner is 8.84 cm/s. Note that the unbounded flame has a burning velocity of more than 250 cm/s (see Table 2).

To model a burner stabilized flame, we assume that the species cannot diffuse back into the burner. Then the mass flux fractions of the species at the burner surface must be preserved. This is the boundary condition for each species.[22,5] A similar condition for the heat flux can be used for the temperature profile. However, it is simpler just to specify the temperature at the burner surface. Also, we assume that hydrogen atoms recombine on the burner surface to form H_2.[22]

When Cattolica et. al. modeled this flame, they used the experimental temperature profile and only solved for the species profiles. The rationale was that the heat loss was too complicated to model accurately. One difficulty is that the temperature profile can not be measured near the burner. Cattolica used a straight line to approximate the temperature profile

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[22]J. Warnatz, "Calculation of the Structure of Laminar Flat Flames III: Structure of Burner-Stabilized Hydrogen-Oxygen and Hydrogen-Fluorine Flames," Ber. Bunsenges. Phys. Chem. Vol 82, pp. 834-841, 1978.

between the burner (assumed 1000K) and the first measured temperature point (around 1900K). This will lead to inaccuracies in the early part of the flame.
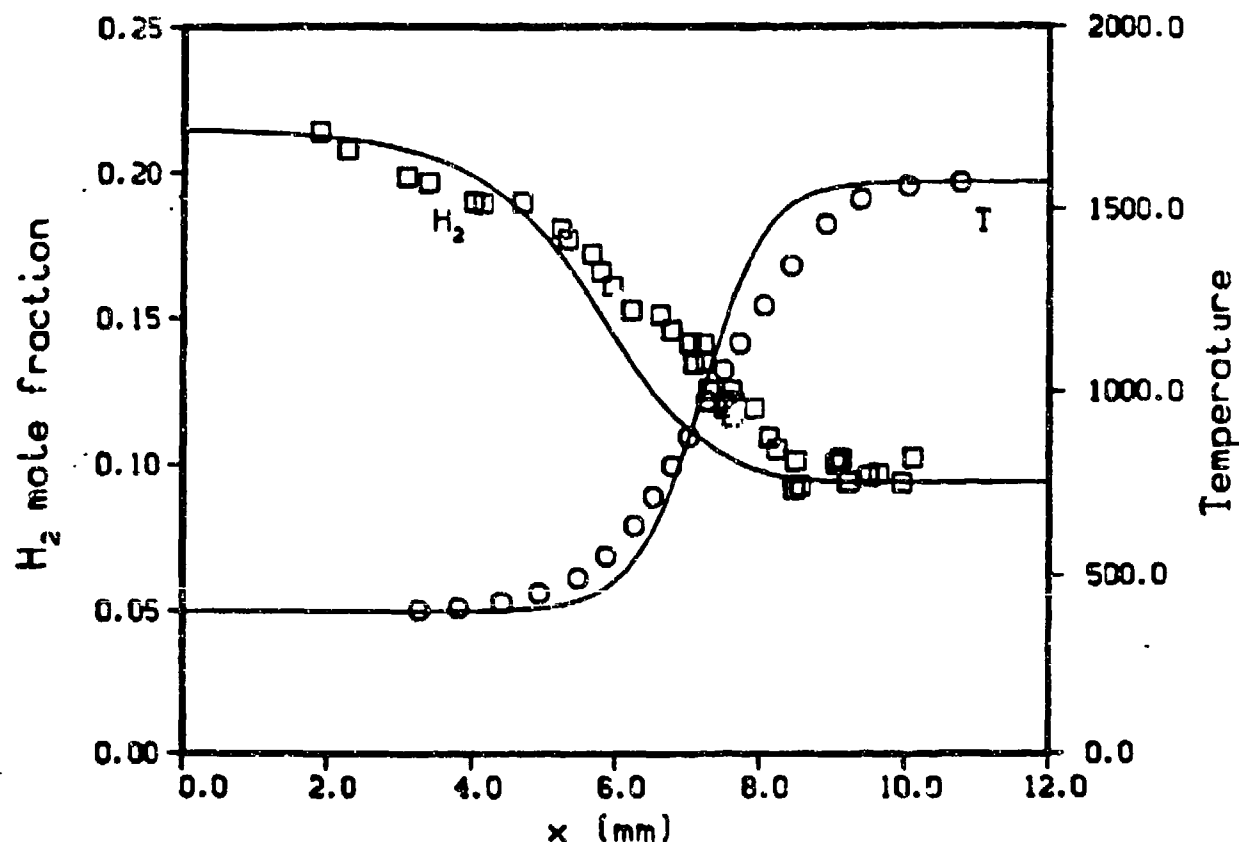

Figure 1. Dixon-Lewis Flame, Last Case, Table 4.

In our code, we did solve for the temperature profile, using the boundary condition that the temperature at the burner was 1000K. The temperature agreement is good nearer the burner, but the model temperature is noticeably higher than the experimental temperature (around 150K) further from the burner, probably because of heat loss to the surrounding air due to conduction or radiation (see fig. 2).

Now consider the species profiles in fig. 2. The NH and NO profiles are fairly accurate. The OH profile is much too large. This could be partially due to the neglect of heat loss, since a cooler flame would have lower radical
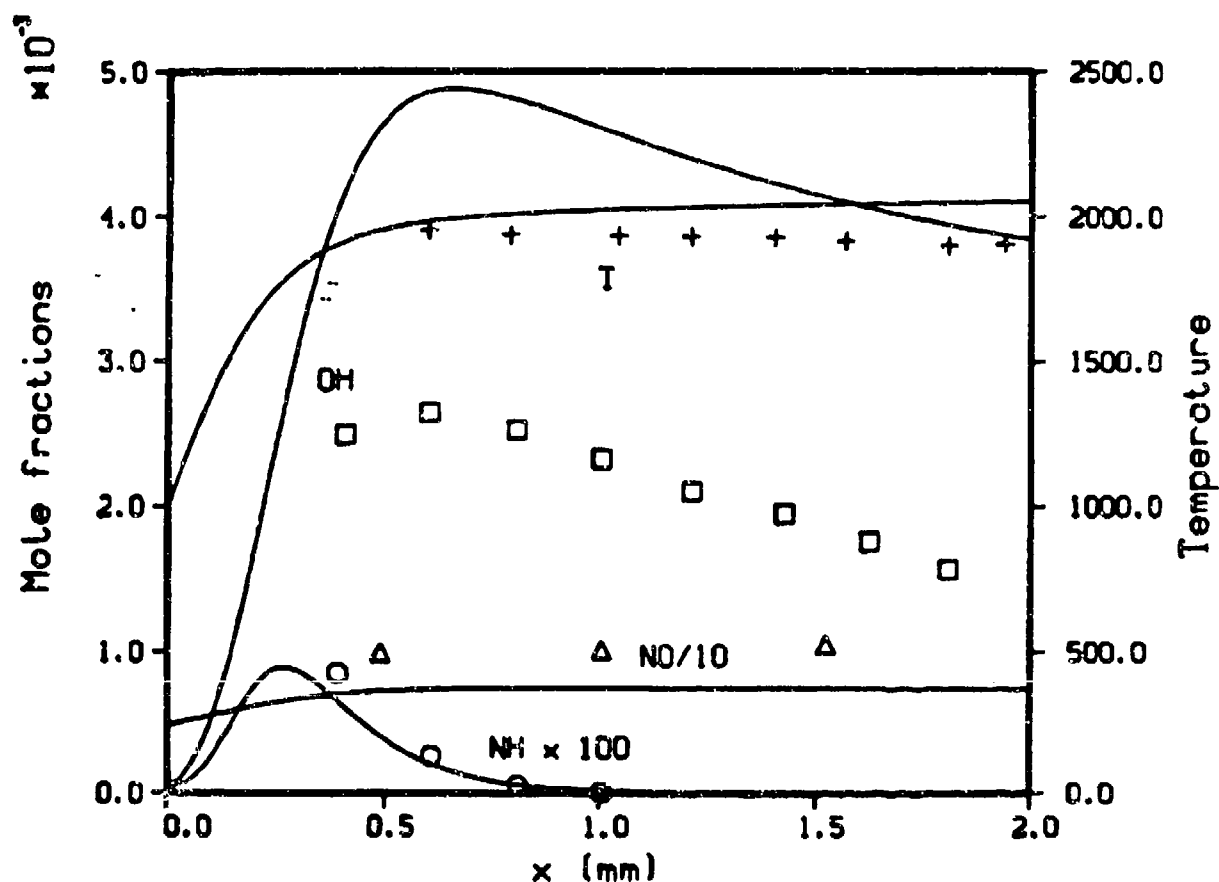
concentrations.

Figure 2. Cattolica, Smooke, and Dean Flame.

To check on the effect of the heat loss, we solved the problem using Cattolica's temperature profile. The OH peak was lower, but only by about 10%. The NH and NO profiles showed larger differences (20% to 30%). We also solved the problem using the model temperature profile for the lower temperatures and Cattolica's experimental profile only in the regime where the temperature was actually measured. In this case, the OH profile was still almost 10% lower, but the NH and NO profiles were almost identical with our original computation. So using a linear approximation for the temperature profile over such a wide temperature range may lead to inaccuracies in some species profiles.

An additional problem is the contribution that the boundary conditions at the burner have on the profiles. The model OH profile for the corresponding unbounded flame is ten times as large as the model profile for the stabilized flame. While our algorithm for computing diffusion coefficients is quite accurate,[2] it may not be accurate enough to properly determine the boundary conditions.

Vanderhoff et. al. has measured NO, O_2, N_2, and temperature profiles for three lean hydrogen/nitrous oxide flames using Raman spectroscopy.[23] They also measured relative OH profiles using laser fluorescence. The burner conditions are essentially equal to those of Cattolica.[1]

Results for a flame with $\phi = 0.89$ is shown in fig. 3. The OH profile is not shown, since we do not have an absolute value. The model agrees fairly well with the experimental data. The other two flames show similar agreement.

Absolute OH concentrations, along with the corresponding temperatures, have been measured by Decker and Kotlar[24] using laser absorption techniques.[25,26] The experiment was done on a knife edge burner[27] so heat loss to the burner is negligible. The flame is rich ($\phi = 1.17$) and heavily diluted with argon (67%). The temperatures are used to locate the position of the measured values in the model OH profile. The results are shown in fig. 4.

[23] J.A. Vanderhoff, S.W. Bunte, A.J. Kotlar, and R.A. Beyer, "Temperature and Concentration Profiles in H2/N2O Flames," to be published in Combustion and Flame.

[24] L.J. Decker and A.J. Kotlar, private communication, 1984.

[25] W.R. Anderson, L.J. Decker, and A.J. Kotlar, "Temperature Profile of a Stoichiometric CH4/N2O Flame form Laser Excited Flourescence Measurements on OH," Combustion and Flame Vol 48, pp. 163-176, 1982.

[26] W.R. Anderson, L.J. Decker, and A.J. Kotlar, "Concentration Profiles of NH and OH in a Stoichiometric CH4/N2O Flame by Laser Excited Flourescebce and Absorption," Combustion and Flame Vol 48, pp. 179-190, 1982.

[27] R.A. Beyer and M.A. DeWilde, "Simple Burner for Laser Probing of Flames, " Rev. Sci. Instrum. Vol 53(1), pp. 103-104, 1982.
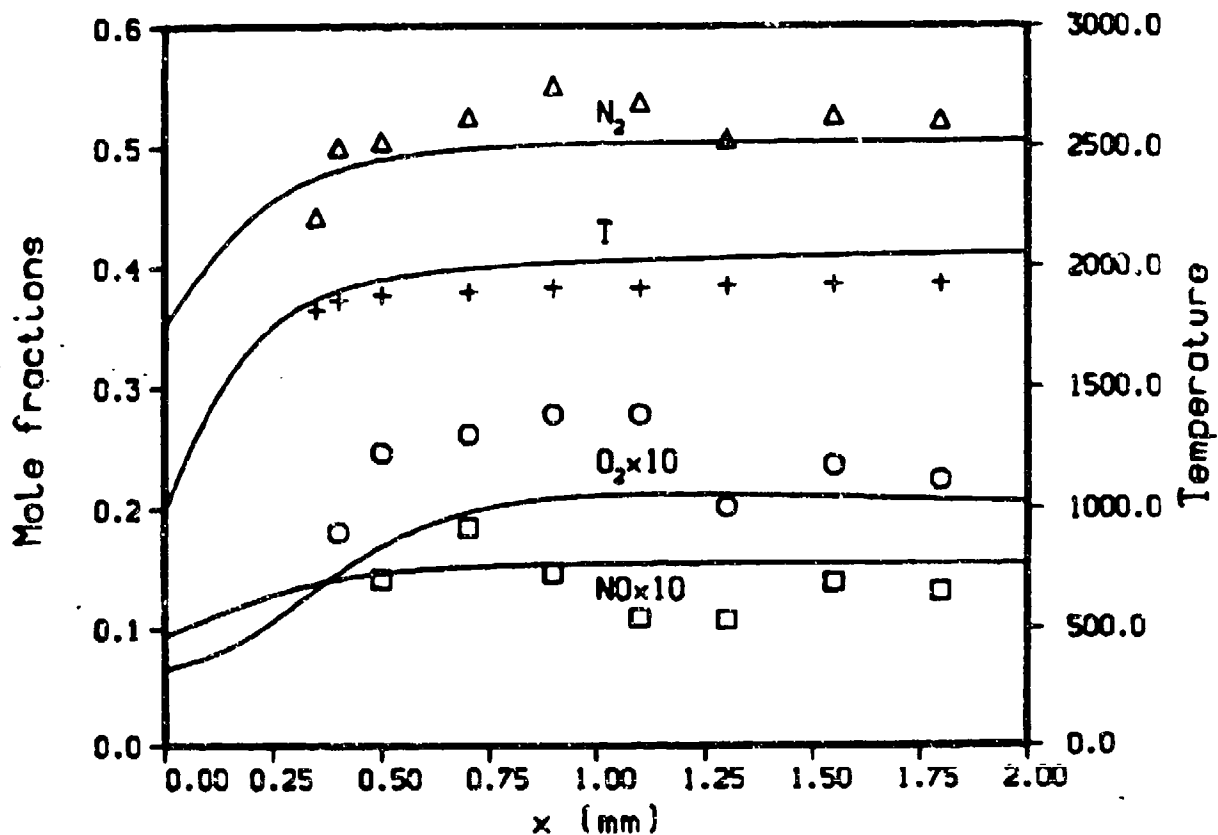
Figure 3. Vanderhoff et. al. Flame.

Unlike Cattolica's measurement, the model OH profile is slightly smaller than the experimental data. However, Cattolica's flame was an undiluted fast flame with a large heat loss to the burner. This flame is a dilute slower flame ($S_M = 31$ cm/sec) with negligible heat loss. This makes it difficult to conclude that the two experiments contradict each other.

V. SENSITIVITY ANALYSIS

A sensitivity analysis was performed for a lean flame ($X_{H2} = .23$, $X_{N2O} = .345$); a stoichiometric flame ($X_{H2} = .25$, $X_{N2O} = .25$); and a rich flame ($X_{H2} = .39$, $X_{N2O} = .21$). The larger logarithmic sensitivity coefficients S_E^1 for the burning velocities are given in Table 5. These are defined such that if the

rate of the reaction is changed by a small factor α, the burning velocity will change by α to the S_E^i power. Analytically, the sum of the S_E^i must equal 0.5. [28]
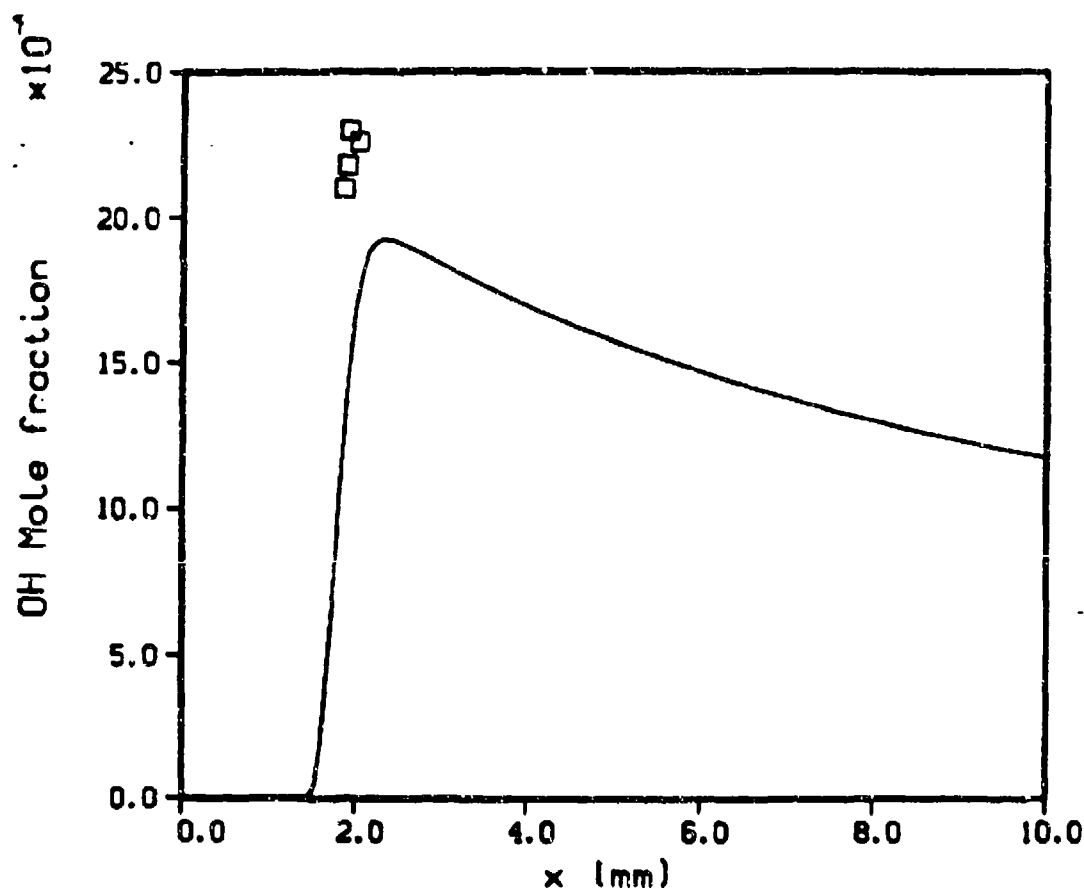

Figure 4. Decker and Kotlar Flame.

The flame is most sensitive to the reactions that break up the N_2O, that is, reaction 14 ($N_2O + H \rightarrow N_2 + OH$) and reaction 16 ($N_2O + M''' \rightarrow N_2 + O + M'''$). The only other reaction that is very important is reaction 1 ($OH + H_2 \rightarrow H_2O + H$). Unlike flames with O_2 as an oxidizer,[7,18,19,22] the chain branching reactions 2 and 3 are not very important.

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[28]T.P. Coffee and J.M. Heimerl, "Sensitivity Analysis for Preximed, Laminar, Steady State Flames," Combustion and Flame, Vol 50, pp. 323-340, 1983.

TABLE 5.   LOGARITHMIC SENSITIVITY COEFFICIENTS FOR BURNING VELOCITIES

Reaction	lean	stoichiometric	rich
1	.14	.07	.02
3	.04	.01	.00
9	-.01	-.02	-.03
12	-.06	-.02	-.00
14	.24	.32	.36
15	-.02	-.04	-.05
16	.19	.18	.23
17	-.01	-.01	-.03

Sensitivity coefficients for the species and temperature profiles were also computed (as a function of position). The temperature and major species (N_2O, H_2, H_2O, and N_2) are fairly insensitive to changes in the reaction rates. In general, the lower the concentration of the species, the more sensitive it is to changes in the chemistry.

Consider the species measured by Cattolica et. al. The OH profile is primarily sensitive to reactions 14 (N_2O + H → N_2 + OH) and 16 (N_2O + M''' → N_2 + O + M'''). If either of these rates are increased, the OH concentration will increase. This correlates with the sensitivity coefficients for the burning velocity. An increase in reaction 15 (N_2O + H → NO + NH) will decrease the OH concentration slightly, since this is an alternate pathway for the breakup of N_2O.

For the NH and NO profiles, reaction 15 (N_2O + H → NO + NH) is important. While this reaction does not decompose very much of the N_2O, it does lead directly to the species NO and NH, and is important in determining their concentrations. If the competing reaction 14 is increased, the NH and NO concentrations are decreased. If the competing reaction 16 is increased, the NH concentration will decrease, but the NO concentration will increase. This is because some of the O created by reaction 16 goes to NO by reaction 12 (N_2O + O → NO + NO). Reaction 12 is most important in lean flames, where there is an excess of oxidizer. So the sensitivity for the species profiles is slightly more complicated than the sensitivity for the burning velocity.

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To help analyze the results, a screening analysis is performed.[29]   That
is, the rate of production and loss for each species as a function of position
is partitioned according to the contribution of each reaction. This shows the
pathways by which the various species are produced and consumed in a given
network. Screening analysis compliments a sensitivity analysis, which shows
how changes in the rates can affect the given network.

For most of the flames, 95% of the N_2O is consumed by reaction 14 (N_2O +
H → N_2 + OH). The OH produced is consumed almost entirely by reaction 1 (OH +
H_2 → H_2O + H). So a very simple 2 step mechanism describes the main structure
of the chemistry in the flame. Reaction 16 (N_2O + M''' → N_2 + O + M''') only
becomes important in the faster .therefore hotter) flames, since it has a very
high activation energy. But it still only consumes around 15% of the N_2O.
Nevertheless, the sensitivity analysis shows that if this rate is increased
even moderately, it will become more important.

So it seems that either the rate for reaction 14 or for reaction 16 must
be increased to match the experimental burning velocities. Since the third
body efficiencies for reaction 16 are not well known, this seems the most
likely place for errors in the rate constants. The two cases where the model
burning velocities are greater than the experimental burning velocities cannot
presently be explained.

Next consider the profiles in Fig. 2. Cattolica et. al. [1] increased
reaction 15 by a factor of two in order to improve the agreement in the
species profiles. This would decrease the OH concentration and increase the
NO concentration, which is what is required. However, this would decrease the
OH profile in fig. 4, and also decrease the burning velocities. We have
solved a few of the flames from Table 2 using the Cattolica model and the
burning velocities were substantially smaller than those reported in this
paper.

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[29]R.J. Gelinas, "Ignition Kinetics of C1 and C2 Hydrocarbons," Science
Applications, Inc., Preprint No. SAI/PL/C279, December 1979.

At present, we cannot adjust the rates to match both the burning velocity measurements and the profile measurements of Cattolica et. al. The difficulty is probably due to the fact that the flame measured by Cattolica is so strongly stabilized. The interaction with the burner decreases the burning velocity of the flame and the OH concentration by at least an order of magnitude. While the experimental values can be measured adequately, the flame model is probably inadequate to properly resolve the complicated behavior at the burner surface.

VII. CONCLUSIONS

The model reported here and the earlier model by Cattolica et. al.[1] both describe the basic characteristics of H_2/N_2O flames. The combustion can be explained as occurring primarily through the two reactions 14 and 1. Beyond this, the combustion is not well understood.

From the analysis in this paper, the most important reactions are 14, 1, 16, and 15. Of these reactions, the third body efficiencies for reaction 16 and the rate for reaction 15 are not well known. Obtaining better values for these rates is quite important in deciding the adequacy of the above kinetics scheme.

In any case, the validation of the reaction network is hindered by a lack of experimental data. Measurements of burning velocity over a range of stoichiometries, using reliable methods,[16] would be the most useful. If the model matches the burning velocities, it will generally also match the temperature and major species profiles. Measurements of temperature and major species profiles are less helpful as diagnostics.

Absolute measurements of radical species profiles are useful for validating the details of the kinetics. The OH and NO profiles seem to be the most important. It is preferable to measure these in a case where the flame is not strongly stabilized against a burner, so the boundary conditions at the burner surface are not so critical.

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